

# The algorithm for simulating of phase transition in Ising magnetic

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Simple algorithm of dynamics of Ising magnetic is described. The algorithm can be implemented on conventional digital computer and can be used for construction of specialized processor for simulation of ferromagnetic systems. The algorithm gives a simple way to calculate 1D correlation functions for 1D Ising magnetic.

## I. INTRODUCTION

In recent past the analog computers were the only tool for solving the mathematical problems which could not be solved analytically. The analog computer is a device (typically - an electric circuit) whose temporal dynamics is described by equations similar to those which are to be solved. The analog computers have the virtue of being simple. The main defect of analog computers is absence of universality. For this reason for solving of any particular problem one must design a special analog computer suited for solving only this particular problem. The impressive achievements of semiconductor technology of recent decades made it possible to create a digital universal computer based on microprocessor - a programmable electronic device which is millions times more complicated than any of analog computers but allows one to solve wide range of problems just by entering of appropriate program. Despite the great power of modern digital universal microprocessors one can point out some problems whose solution require excessive time or even impossible. Having in mind one of these problems one can put the following question: is it possible (using the fantastic facilities of up-to-date technology) to create a specialized device (specialized processor) suited for solving only this particular problem? Imagine that we have constructed the specialized processor for solving of many-particle problem of atomic physics. In our opinion despite the loss of universality this processor would be of great interest. Below we suggest some algorithm for solving the problem of phase transition in Ising magnetic. This algorithm can be directly implemented by means of conventional digital computer. On the other hand in our opinion it is quite possible to create the specialized processor working according to this algorithm but much faster than conventional universal processor. This processor being much more simple device than the universal processor allows one to solve the problem of phase transition in Ising system and to obtain an arbitrary values of interest (energy, magnetisation, heat capacity). We estimate the complexity of this processor to be comparable with that of modern memory devices.

Let us consider a trigger - scheme with two stable states which we denote by  $\pm 1$ . This trigger and spin  $1/2$  have much in common and below we will not differ these two. Suppose this trigger can change its state only when clock pulse coming. We consider the train of clock pulses to be equidistant in time. Consider the probability for trigger to change its state (the probability of corresponding spin flip) be depending on the trigger's state before clock pulse coming. Consequently the probability  $p_+$  for trigger to switch from state  $s = +1$  differs from that  $p_-$  to switch from state  $s = -1$ :  $p_+ \neq p_-$ . Let these probabilities obey:

$$p_{\pm} = \alpha \exp\left(\beta h s\right), \quad s = \pm 1. \quad (1)$$

Equation (1) has the sense of detail equilibrium principle for spin  $1/2$  in magnetic field  $h$

and in contact with thermostat with inverse temperature  $\beta$ . Since  $p_{\pm} \leq 1$  the normalization constant  $\mathfrak{x}$  must obey:

$$\mathfrak{x} \leq \exp \left( -\beta|h| \right) \quad (2)$$

If we now consider the statistical ensemble of such triggers then the kinetic equations for average number  $n_{\pm}$  of triggers in states  $\pm 1$  have the form:

$$\begin{aligned} \Delta n_+^i &= -n_+^i p_+ + n_-^i p_- \\ \Delta n_-^i &= -n_-^i p_- + n_+^i p_+ \end{aligned} \quad (3)$$

where  $\Delta n_{\pm}^i$  – is increment of number of triggers in state  $s = \pm 1$  after  $i$ -th clock pulse coming,  $n_{\pm}^i$  – number of triggers in state  $s = \pm 1$  to the moment of  $i$ -th clock pulse coming.

The steady state solution of this equation has the form:

$$\frac{n_+^{st}}{n_-^{st}} = \frac{p_-}{p_+} = \exp \left( -2\beta h \right) \quad (4)$$

This corresponds to thermal equilibrium state of spin system in the external magnetic field  $h$ .

Now let us consider the case of Ising magnetic i.e. the lattice comprised of  $N$  spins (triggers) coupled to each other in such a way that the magnetic field acting on the arbitrary spin is defined by configuration of the rest spins in the lattice. In the simplest case the magnetic field  $h_i$  acting on spin with number  $i$  is produced by its nearest neighbours and if we denote the set of nearest neighbours by  $nn(i)$  then:

$$h_i = W \sum_{r \in nn(i)} s_r, \quad (5)$$

here the constant  $W$  characterize interspin coupling. By the analogy with the aforesaid let us consider the following dynamics of this system. The clock pulses act sequentially on all the spins (triggers) in the lattice – we call this *round trip*. During the round trip any spin (say  $i$ -th) may be overturned with probability defined by equation (1) with magnetic field  $h_i$  defined by formula (5). We are interesting in the dynamics of this system under the action of the train of round trips. For the above dynamics of this "Ising magnetic" (consisting of triggers controlled by clock pulses) we now will obtain the kinetic equation for density matrix and will show that its steady state solution corresponds to thermal equilibrium. By the analogy with real magnetic let us describe the state of our "magnetic" (consisting of triggers) by the wavefunction whose  $i$ -th argument describe the state of  $i$ -th spin (trigger):

$$\Psi = |s_1, s_2, \dots, s_N\rangle \quad (6)$$

Introduce  $\hat{O}_i$  – operator of  $i$ -th spin flip:

$$\hat{O}_i |s_1, s_2, \dots, s_i, \dots, s_N\rangle = |s_1, s_2, \dots, -s_i, \dots, s_N\rangle \quad (7)$$

Let us introduce the statistical ensemble of Ising magnetics and let  $\sigma(\Psi)$  be the number of magnetics in state  $\Psi$  in this ensemble. Up to normalization factor the quantities  $\sigma(\Psi)$  are represent the diagonal elements of the density matrix of Ising magnetic. Let us consider  $\Delta\sigma^i$  – the increment of  $\sigma$  when clock pulse act on  $i$ -th spin (trigger)

$$\Delta\sigma^i(\Psi) = - \sum_{\Phi \neq \Psi} \sigma(\Psi) V_{\Psi \rightarrow \Phi} + \sum_{\Phi \neq \Psi} \sigma(\Phi) V_{\Phi \rightarrow \Psi} \quad (8)$$

Here  $V_{\Psi \rightarrow \Phi}$  – is the probability of transition from  $\Psi$ -state to  $\Phi$ -state when clock pulse act on  $i$ -th spin. In accordance with the above dynamics of Ising magnetic the only non-zero probabilities are:

$$(\text{probability of transition from } \Psi \text{ to } \Phi = \hat{O}_i \Psi) = \mathfrak{x} \exp \left( \beta h_i(\Psi) s_i(\Psi) \right) \quad (9)$$

$$\begin{aligned} (\text{probability of transition from } \Phi = \hat{O}_i \Psi \text{ to } \Psi) &= \mathfrak{x} \exp \left( \beta h_i(\Phi) s_i(\Phi) \right) = \\ &= \mathfrak{x} \exp \left( - \beta h_i(\Psi) s_i(\Psi) \right) \end{aligned} \quad (10)$$

The last equality follows from the fact that the field acting on  $i$ -th spin in states  $\Phi = \hat{O}_i \Psi$  and  $\Psi$  is the same while the value of  $i$ -th spin has the opposite sign (i.e.  $s_i(\Phi = \hat{O}_i \Psi) = -s_i(\Psi)$ ). Then using equation (8) one can see that

$$\Delta\sigma^i(\Psi) = \mathfrak{x} \left[ \sigma(\hat{O}_i \Psi) \exp \left( - \beta h_i(\Psi) s_i(\Psi) \right) - \sigma(\Psi) \exp \left( \beta h_i(\Psi) s_i(\Psi) \right) \right] \quad (11)$$

Let us show that this equation has the steady state solution in the form:

$$\sigma_{eq}(\Psi) = \exp \left( \lambda H(\Psi) \right) \quad (12)$$

where  $H$  – is the Hamiltonian of Ising magnetic:

$$H = \frac{W}{2} \sum_{i=1}^N \sum_{\alpha=nn(i)} s_i s_\alpha \quad (13)$$

We need to calculate  $\sigma_{eq}(\Phi = \hat{O}_i \Psi)$ . To do this note that:

$$H(\Phi = \hat{O}_i \Psi) = H(\Psi) - 2W \sum_{\alpha=nn(i)} s_i s_\alpha \Big|_{\Psi} = H(\Psi) - 2h_i(\Psi) s_i(\Psi) \quad (14)$$

Now calculating  $\sigma_{eq}(\Phi = \hat{O}_i \Psi)$  by equation (12) and substituting the result in to equation (11) it is easy to see that when  $\lambda = -\beta$  the right part of equation (11) vanishes. So we see that (12) is the steady state solution of (11) and represent thermal equilibrium density matrix of Ising magnetic. Thus the above algorithm of sequential round trips prepare the system of coupled triggers in thermal equilibrium state. For transition probabilities be less than unit the value of  $\mathfrak{x}$  should obey:

$$0 \leq \mathfrak{x} \leq \exp \left( - \beta m |W| \right), \quad (15)$$

here  $m$  – is the number of nearest neighbours. In our opinion it is possible to create a specialized processor working in accordance with this algorithm. The described algorithm can be implemented on conventional digital computer. In this case  $\mathfrak{x}$  should take the maximum possible value  $\mathfrak{x} = \exp \left( - \beta m |W| \right)$  for system to relax as fast as possible.

In relaxed system one can observe magnetisation  $S = \sum_i s_i$ , energy (13), heat capacity  $c = \partial \langle H \rangle / \partial T$ , an arbitrary correlation functions.

To demonstrate the aforesaid algorithm we simulate the phase transition in two-dimensional Ising magnetic by means of conventional computer. Fig.1 shows the temperature dependence of heat capacity (top), magnetisation (middle) and energy (bottom) calculated for the case of  $W = -1$  (ferromagnetic). Calculations were performed for lattice with sizes  $1000 \times 1000$ . The procedure was as follows. At the beginning the system was prepared in the state with magnetisation close to its ultimate value  $S = N$  and with temperature much lower than the temperature of phase transition  $T_c$ . After that the above algorithm started with gradually increasing temperature  $1/\beta$ . When temperature becomes close to  $T_c$  the magnetisation vanishes and heat capacity takes its maximum value. The value of  $T_c$  obtained in our calculations is in agreement with the exact formula of Kramers and Wannier [1].

The similar calculations can be performed for the case of *zero* initial magnetisation  $S = 0$ . In this case total magnetisation is zero for all temperatures. Fig.2 shows the spatial distribution of 2D magnetisation below  $T_c$  (top picture, the domains are clearly seen) and above  $T_c$  (bottom). The heat capacity and energy temperature behaviour is similar to that in fig.1.

The algorithm described can be directly generalized for the case of Ising system with an arbitrary interspin interaction  $W(r)$ :

$$H = \frac{1}{2} \sum_{ik} W(i-k) s_i s_k$$

To do this one should use the effective magnetic field in the form

$$h_i = \sum_r W(r-i) s_r$$

instead equation (5).

Possibly the described algorithm may be useful for checking the gauge theories of critical phenomena [3, 4, 5]. In this case the duality of some gauge models with respect to Ising system is exploited. The similar algorithms were described in [3, 4, 5].

## II. 1D- CORRELATION FUNCTIONS.

To check the above algorithm let us consider the exactly solvable one-dimensional Ising magnetic with nearest neighbours interaction. This problem was solved by Ising [2] but above algorithm provide a simple way to obtain formulas (27) for correlation functions which are not very popular. In the case of 1D Ising magnetic with nearest neighbours interaction the field acting on the  $i$ -th spin can be calculated by formula (5) as:

$$h_i = W(s_{i-1} + s_{i+1}) \quad (16)$$

Suppose the clock pulse acts on  $i$ -th spin (trigger). Let us calculate the increment  $\Delta \langle s_i f \rangle$ , where  $f$  is an arbitrary function of all spin variables except  $s_i$ . Multiplying both parts of equation (11) by  $s_i f$  and summing over all states  $\Psi$  we obtain:

$$\Delta \langle s_i f \rangle = \text{æ} \left( - \sum_{\Psi} \sigma(\Psi) f s_i \exp[\beta W(s_{i+1} + s_{i-1}) s_i] \right) \Big|_{\Psi} \quad (17)$$

$$+ \sum_{\Psi} \sigma(\hat{O}_i \Psi) f s_i \exp[-\beta W(s_{i+1} + s_{i-1}) s_i] \Big|_{\Psi} \Big)$$

Passing from summation over  $\Psi$  to summation over  $\hat{O}_i \Psi$  in the second sum ( $s_i$  should be replaced by  $-s_i$ ), denoting

$$\beta W \equiv \theta, \quad (18)$$

and using the relation

$$\exp \alpha s = \text{ch } \alpha + s \text{ sh } \alpha, \quad s = \pm 1, \quad (19)$$

we obtain:

$$\begin{aligned} \Delta \langle s_i f \rangle &= -2\mathfrak{e} \langle f s_i \exp[\beta W(s_{i+1} + s_{i-1}) s_i] \rangle = \\ &= -2\mathfrak{e} \left( \text{ch}^2 \theta \langle s_i f \rangle + \frac{1}{2} \text{sh} 2\theta (\langle s_{i+1} f \rangle + \langle s_{i-1} f \rangle) + \text{sh}^2 \theta \langle s_{i+1} s_i s_{i-1} f \rangle \right) \end{aligned} \quad (20)$$

Hence in the equilibrium state:

$$\text{ch}^2 \theta \langle s_i f \rangle + \frac{1}{2} \text{sh} 2\theta (\langle s_{i+1} f \rangle + \langle s_{i-1} f \rangle) + \text{sh}^2 \theta \langle s_{i+1} s_i s_{i-1} f \rangle = 0 \quad (21)$$

Now we use this relationship to calculate the equilibrium correlation function:

$$k_p \equiv \langle s_i s_{i+p} \rangle. \quad (22)$$

This function depends only on the difference  $p$  of its indexes. Let  $f = s_{i+p}$  in equation (21). Then we have:

$$k_p \text{ch}^2 \theta + \frac{1}{2} (k_{p+1} + k_{p-1}) \text{sh} 2\theta + \text{sh}^2 \theta \langle s_{i+1} s_i s_{i-1} s_{i+p} \rangle = 0 \quad (23)$$

To calculate the correlation function entering the last term let  $f = s_{i+1} s_{i-1} s_{i+p}$  in equation (21). We have:

$$\text{ch}^2 \theta \langle s_{i+1} s_i s_{i-1} s_{i+p} \rangle + \frac{1}{2} (k_{p+1} + k_{p-1}) \text{sh} 2\theta + k_p \text{sh}^2 \theta = 0 \quad (24)$$

Hence:

$$\langle s_{i+1} s_i s_{i-1} s_{i+p} \rangle = -k_p \text{th}^2 \theta - [k_{p+1} + k_{p-1}] \text{th} \theta. \quad (25)$$

By substituting (25) in to (23) one can obtain:

$$k_p = \xi (k_{p+1} + k_{p-1}), \quad \xi \equiv -\frac{1}{2} \text{th}(2\theta) \quad (26)$$

The solution of this equation under condition  $k_0 = 1$  has the form:

$$k_p = \exp(\alpha p), \quad \xi > 0, \text{ (ferromagnetic)} \quad (27)$$

$$k_p = (-1)^p \exp(\alpha p), \quad \xi < 0, \text{ (anti-ferromagnetic)}$$

with  $\alpha$  (for  $p > 0$ ) being the negative root of the equation:

$$\text{ch} \alpha = \frac{1}{2|\xi|} \quad (28)$$

Formulas (27) were verified by direct computer simulation according to the above algorithm for 1D Ising magnetic.

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